TWO-ELECTRON QUASI-ONE-DIMENSIONAL NANORING

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ABSTRACT

Energy levels of two-electron confined in quantum ring whose height and width are considerably smaller than the interior diameter are studied. The adiabatic procedure is used in order to decouple the fast electron motion in z direction from the slow in-plane motion. A one-dimensional wave equation with periodic boundary conditions which describes the two-electron rotation around the axis and gives all low-lying two-electron levels is derived. We show that as the ring height and width tend to zero it gives the results in a good accordance with those obtained previously for the model of a one-dimensional nanoring by using a different method.

Introduction.

The Stranski-Krastanov method has allowed to manufacture zero-dimensional structures called self-assembled quantum dots (QDs) which are expected to provide the base for future generations of device technologies such as threshold-less lasers and ultra-dense memories [1]. InAs/GaAs QDs fabricated by this method can have disk, lens, ring or cone shape with circular top view cross section and a large area-to-height aspect ratio [2], particularly, quantum rings (QRs) whose outer radius is between 30 and 70 nm, inter radius is about 10nm and the height is between 2 and 4 nm [3]. QDs containing one, two or more electrons can be considered as artificial atoms where the confining potential replaces the nucleus. The spectrum of these artificial atoms is determined by the interplay between the binding forces due to the confinement and the repulsion between the electrons. Recently, the analysis of two-electron system in QRs has received a great deal of attention [4]. Different methods and approximations have been used to treat this problem. For instance, in the paper [4] has been considered a one-dimensional exactly solvable model, in which the motions in radial and z-directions are neglected and only the rotation of two electrons is taken into account. We consider that this model is justified only for the infinite barrier potential but if the width and the height of the ring tend to zero the energy levels lift drastically and therefore the finite barrier model in this limit can be considered. In spite of this contradiction, we believe that this exactly model can be used as a starting point to analyze the electronic spectra of a more realistic models of the two-electron QRs. In this work we consider a model of QR whose width and thickness are much smaller than the radius and in framework of the adiabatic approximation we derive for this model the one-dimensional wave equation which describes the low-lying energy levels.

Theory

In our numerical work to analyze the electronic spectrum in two-electron $In_{0.55}Al_{0.45}As/Al_{0.35}Ga_{0.65}As$ QR with conduction band offset $V_{off} = 258meV$, for mathematical convenience we used the same physical parameters in the well and in the barriers corresponding to $In_{0.55}Al_{0.45}As$ system: dielectric constant $\varepsilon = 12{,}71$ and the electron effective mass

$m^* = 0.076 m_0$ [5]. The geometrical parameters for the QR we denote by d, the height, R_i and R_e the interior and outer radii, respectively and we consider a typical situation when $d / R_e << 1$. The last condition permits us to apply the adiabatic approximation and to separate the motions in z and in-plane directions. As it is shown in the paper [6] the two-electron 3D problem in this case can accurately be approximated by a 2D problem in which the barrier height can be renormalized as $V_0 = V_{off} - k_z^2(d, V_{off})$ where $k_z^2(d, V_{off})$ is the lowest energy level in a quantum well of rectangular form with the width d and the barrier height V_{off}. Thus, our two electron system can be accurately described by the effective 2D Hamiltonian in plane polar coordinates is given by:

$$H = H_0(\boldsymbol{\rho}_1) + H_0(\boldsymbol{\rho}_2) + \frac{2}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|}; \; H_0(\boldsymbol{\rho}) = -\frac{1}{\rho}\frac{\partial}{\partial \rho}\rho\frac{\partial}{\partial \rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial \varphi^2} + V(\rho) \qquad (1)$$

where $V(\rho) = 0$ for $R_i < \rho < R_e$ and $V(\rho) = V_0$ for $\rho < R_i$ and $\rho > R_e$. For $In_{0.55}Al_{0.45}As$ material, the effective Rydberg is $Ry^* = 6.40\, meV$ and effective Bohr radius is $a_0{}^* = 8.86\, nm$. The Schrödinger equation for the one-electron problem,

$$H_0(\boldsymbol{\rho}) f_{n,m}(\boldsymbol{\rho}) = E_0(n, m) f_{n,m}(\boldsymbol{\rho}); \quad f_{n,m}(\boldsymbol{\rho}) = e^{im\varphi} R_{n,m}(\rho) \qquad (2)$$

has a solution that depends on two quantum numbers, radial, n and orbital, m. For the piecewise constant function $V(\rho)$ the radial part $R_m(\rho)$ can be found in an analytical form as a combination of the different types of the Bessel functions. The electron-electron interaction in the two-electron system provides the mixing of the one-electron states in such way that the mixing of the different groups of the sublevels is depreciable in comparison with the mixing of the sublevels inside the groups. Therefore the low-lying two-electron levels are form by mixing of only sublevels with the radial quantum number $n = 1$. On the other hand, one can see that the radial parts of the one-electron wave functions $R_{1,m}(\rho)$ for different orbital quantum number m are similar and therefore all of them in the variational calculation for the two-electron QR can be approximated by the same radial part wave function $R_{1,0}(\rho)$. It is the reason why we propose the following trial wave function for the low-lying states:

$$\psi(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) = R_{1,0}(\rho_1) R_{1,0}(\rho_2) \Phi(\varphi_1, \varphi_2) \qquad (3)$$

where the variational function $\Phi(\varphi_1, \varphi_2)$ describes the two-electron system angular motion corresponding to different angular momentum. To derive a differential equation for the unknown function $\Phi(\varphi_1, \varphi_2)$ we use the Schrödinger variational principle which states that eigenfunction of the Hamiltonian H should minimize the functional $F[\Phi] = \langle \psi | H - E | \psi \rangle$. Substituting (3) and (1) in this functional and taking the functional derivative with respect the function Φ we obtain after some algebraic manipulation the following wave equation for this function:

$$-\frac{1}{I}\left(\frac{\partial^2\Phi}{\partial\varphi_1^2}+\frac{\partial^2\Phi}{\partial\varphi_2^2}\right)+\tilde{V}(\varphi_1-\varphi_2)\Phi=\left(E-2E_0(1,0)\right)\Phi; \quad (4a)$$

$$\frac{1}{I}=2\pi\int_0^\infty\frac{R_{1,0}{}^2(\rho)}{\rho}d\rho;\ \tilde{V}(\varphi)=8\pi^2\int_0^\infty\rho_1R_{1,0}{}^2(\rho_1)d\rho_1\int_0^\infty\frac{\rho_2R_{1,0}{}^2(\rho_2)}{\sqrt{\rho_1^2+\rho_2^2-2\rho_1\rho_2\cos\varphi}}d\rho_2 \quad (4b)$$

The equation (4) can be separated by using the center-of-mass and relative–motion coordinates, $\vartheta=(\varphi_1+\varphi_2)/2$ and $\varphi=\varphi_1-\varphi_2$ in which the exact solution of the wave equation can be written as:

$$\begin{aligned}&\Phi(\vartheta,\varphi)=e^{iM\vartheta}u(\varphi);\\&u''(\varphi)+\left\{I\left[E/2-E_0(1,0)-\tilde{V}(\varphi)/2\right]-M^2/4\right\}u(\varphi)=0;\\&-2\pi<\varphi<2\pi;\ 0<\vartheta<2\pi\end{aligned} \quad (5)$$

As the effective potential in the wave equation (4) is even, there are two different groups of solutions, even solutions for which $u(-\varphi)=u(\varphi)$ corresponds to singlet states and odd solutions for which $u(-\varphi)=-u(\varphi)$ corresponding to triplet states. Below we consider only the singlet states, for which also it should aggregated the following periodic condition [4], $u(\varphi\pm2\pi)=(-1)^M u(\varphi)$, which permits us to considerate the eigenvalue problem (5) only inside the region $0<\varphi<2\pi$ with the boundary conditions, $u'(0)=u'(2\pi)=0$. To solve this eigenvalue problem we use the trigonometric sweep method [7] and find numerically the two-electron QR energy $E(M,m)$ that depends on two quantum numbers, the angular momentum of the center of mass *M* and of the relative motion *m*.

Results

First, to check the accuracy of our numerical procedure we perform the calculations of the energies of some low-lying states in the limiting case as the height and the width of QR tend to zero and the barrier height tend to infinity. In all cases we found a good concordance of our calculations with those obtained in the paper [4]. In Fig.. 2 we present the results for some low-lying singlet state energy levels $E(M,m)$ of two electrons in In0.55Al0.45As/Al0.35 Ga0.65As QR's with different interior radii, R_i, widths, R_e-R_i, and heights, d. Following to the paper [4] we use in these figures for the sake of convenience the normalized energies defined as $E_{norm}(M,m))=[E(M,m)-2E_0(1,0)]\cdot R_0^2$, where $R_0=(R_i+R_e)/2$. In Fig. 1 we present the energies of the some low-lying states as a function of the interior radius as the height d and width R_e-R_i of QRs are fixed and both are equal to 2nm in the first case (Fig. 1a) and to 4nm and 5nm, respectively in the second case (Fig.1b). In both cases the ground state level always is separated from the other low-lying levels independently of the QR's radius and for other low-lying levels it is observed the crossovers of the curves related to the strong electron-electron interaction. A change of the level-ordering and crossovers of the curves is more significant as the QR's height and width decreases. It is seen from Fig. 1a that for small QR radii the levels with the same value of M and different values of m are degenerated because of the relative rotation in this case does not give any contribution in the total energy of the two-electron system. On the contrary, for large radii the contribution of the rotation of the center of mass is insignificant and therefore the levels with different values of M and the same values of m tend to the same values of the total energy. As the result the crossovers of the curves are observed in Fig.1a. The above effect disappears as the QR's height and width increase and number of the crossovers as it is seen in Fig. 1b decreases. A difference between curves in Fig.1a and Fig. 1b in the major part is related to the different the renormalized barrier height for two different ring thickness, which are equals to 12.6Ry* as d = 2nm and to 24.6Ry* as d = 4nm. As the consequence, the effects related to the leaking of the wave function in the barrier regions due to the strong confinement in the first case is significant whereas for d = 4nm this effect is almost depreciable and therefore the behavior of the curves on the Fig. 1b is similar to those from the Ref. [4] obtained for the model with infinite barrier height. One can see that all curves in Fig.1a can be conditionally divided into two groups, lower one which have one minimum and the upper group that have one minimum and one maximum. We ascribe the minimum position to the effect of the leaking of the wave function into repulsive core region while the maximum position can be ascribed to the leaking into exterior barrier region.

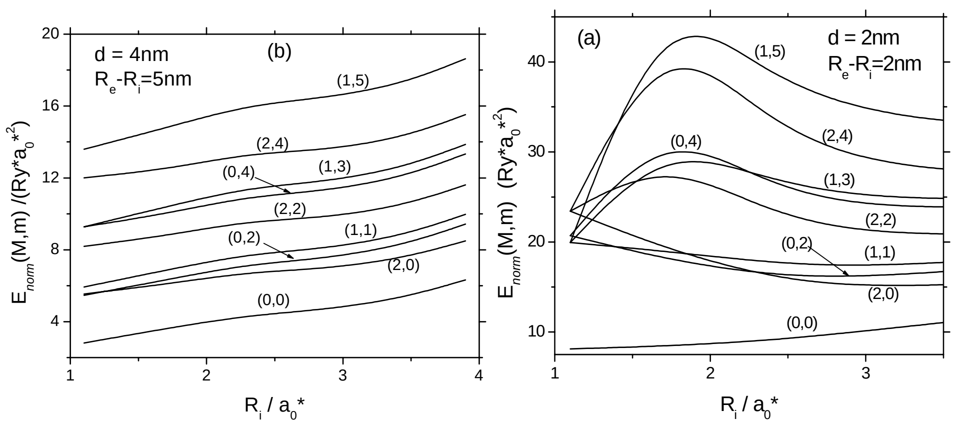

Fig. 1. Normalized energies of the electron-electron interaction as a function of the interior QR radius, R_i for some low lying singlet states in QRs with two different values of the widths, $R_e - R_i$ and heights, d. Notation (M,m) is used for the energy levels E(M,m)

Conclusions

We propose a simple method for calculating the low-lying levels of the two-electron quantum rings with finite thickness and finite barrier height. By using the adiabatic approximation we show that all low-lying levels are related to the center of mass and relative in-plane rotation of two electrons and the one-dimensional wave equation which describes these motions is reduced. We show that that as the thickness and width of the ring tend to zero the effects of the wave function leaking into the central repulsive core and the exterior barrier regions becomes essential produces additional change in the level-ordering and the crossovers of the curves of the two-electron energies as a function ring radius, width and thickness.

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